TORSIONAL SPLITTING AND FOUR-FOLD BARRIER TO INTERNAL ROTATION: THE ROTATIONAL SPECTRA OF VINYLSULFUR PENTAFLUORIDE

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The rotational spectra of vinylsulfur pentafluoride, and three isotopologues (S-34 and both C-13's) have been recorded in the frequency region of 6 GHz to 20 GHz. Measurements were made using both cavity and chirped pulse Fourier transform microwave spectrometers. The four-fold barrier to the internal rotation of the $-SF_5$ group against the vinyl group has been approximated from the spectral data which is possible due to the observation of easily resolved pure rotational transitions in each of the A, B, and doubly degenerate E torsional substates. All transitions were successfully fit simultaneously using the ERHAM code. We note that this work, we believe, represents the first use of pure rotational spectroscopy to characterize a four-fold barrier internal rotation problem. Rotational constants, structure, and the internal rotation barrier height will be presented and compared to results from quantum chemical calculations.